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Particle creation and annihilation at interior boundaries: One-dimensional models

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Abstract. We describe creation and annihilation of particles at external sources in one spatial dimension in terms of interior-boundary conditions (IBCs). We derive explicit solutions for spectra, (generalised) eigenfunctions, as well as Green functions, spectral determinants, and integrated spectral densities. Moreover, we introduce a quantum graph version of IBC-Hamiltonians.

I Introduction

Quantum field theories are plagued by infinities. Among the most serious infinities are ultraviolet divergences. Usually they are taken care of by renormalisation, often within perturbation theory. However, in many cases it is not clear whether the renormalised theory exists at all as a well-defined theory in its own right.

Recently, Teufel and Tumulka proposed a novel formulation of quantum field theory [1], see also [2], where particle creation and annihilation is modelled in terms of conditions coupling Fock space sectors with different numbers of particles. Since such a condition typically relates the n -particle wave function to the value of the $(n+1)$ -particle wave function (or it's derivative) at a specific point, it is called interior-boundary condition (IBC) in Ref. [1]. In simple models the IBC formulation is automatically ultraviolet finite.

In particular, Teufel and Tumulka study models in three spatial dimensions in which non-relativistic scalar particles can be created and annihilated at fixed external sources. These models, when described with the methods of conventional quantum field theory, are known to be renormalisable, even non-perturbatively [3]. The IBC-version turns out to be equivalent to the renormalised theory up to a trivial shift in energy. This correspondence, which is explored in [1], is made mathematically rigorous by Lampart, Schmidt, Teufel and Tumulka [4], see also [5], who show that the relevant IBC-Hamiltonian is essentially self-adjoint and bounded from below. To this end the authors of [1, 4] have to define the domain of the single-particle Hamiltonian such that it contains certain singular functions which are not in the Sobolev space $H^2(\mathbb{R}^3)$. In particular, they allow simple poles at the positions of the sources.

Teufel and Tumulka also give the IBC-formulation of a model with dynamical sources, i.e. a model in which one kind of particles can be created at the positions of particles of a different kind. In a realistic quantum field theory one should think, e.g., of photons

being created at the positions of electrons. It appears that a rigorous non-perturbative analysis of this latter model can be carried out along similar lines as for the model with fixed sources [6].

Conditions similar to IBCs have been studied earlier under the name “zero radius potentials with internal structure”, see e.g. [7] and references therein. In this context they are used to account for rearrangements within a scatterer in diffractive processes. The alternative interpretation of a particle interacting with the vacuum has also been given [8]. This latter interpretation is more in line with the way in which we mainly want to interpret these conditions in the present work.

In this article we study IBCs in one spatial dimension as model systems for which many questions can be answered by explicit calculations. As opposed to the three-dimensional case, we do not have to allow single-particle wave functions with poles but only with kinks. Moreover, one-dimensional IBCs can also be studied on quantum graphs, multiply connected one-dimensional systems, which have become paradigmatic for studies of quantum chaos over the last one and a half decades, see e.g. [9]. The present work thus also introduces model systems for studying quantum chaos in the context of many particle quantum mechanics and quantum field theory.

The article is organised as follows. In Sec. II we motivate the one-dimensional IBC-Hamiltonian as an analogue to the recently introduced IBCs in three dimensions. We introduce versions on both, the full bosonic Fock space and on truncated Fock space with a maximum number of particles. Being interested in the minimal model exhibiting particle creation and annihilation due to interior-boundary conditions, 0-1-particle systems get particular attention in the following sections. In Sec. III we construct a complete orthonormal set of (generalised) eigenfunctions for the IBC-Hamiltonian with one source and determine the corresponding (retarded) Green function. Section IV is devoted to the case of two and more sources. We analyse how the ground state energy depends on the distance of the sources recovering a one-dimensional Coulomb potential for small distances. In Sec. V we discuss the spectrum for one source in a finite box and Dirichlet boundary conditions. Quantum graphs with IBCs in the vertices are introduced in Sec. VI.

II The IBC-Hamiltonian

Before introducing the IBC-Hamiltonian we briefly recall the definition of (bosonic and fermionic) Fock space and particle creation and annihilation operators.

Starting from a one-particle Hilbert space \mathcal{H} , say $\mathcal{H} = L^2(\mathbb{R})$, Fock space is constructed by taking direct sums of tensor products of \mathcal{H} ,

$$\mathcal{F} = \bigoplus_{n=0}^{\infty} \mathcal{H}^{\otimes n}. \quad (1)$$

We represent a vector $\phi \in \mathcal{F}$ as a sequence $\phi = (\phi^0, \phi^1, \phi^2, \dots)$ with

$$\phi^0 \in \mathcal{H}^{\otimes 0} \cong \mathbb{C}, \quad \phi^1 \in \mathcal{H}, \quad \phi^2 \in \mathcal{H} \otimes \mathcal{H}, \dots \quad (2)$$

We symmetrise in order to obtain bosonic Fock space $\mathcal{F}^S = P^S(\mathcal{F}) \subset \mathcal{F}$, where the symmetrisation operator acts on $\phi \in \mathcal{F}$ as

$$(P^S \phi)^n(x_1, \dots, x_n) = \frac{1}{n!} \sum_{\sigma \in S_n} \phi^n(x_{\sigma(1)}, \dots, x_{\sigma(n)}). \quad (3)$$

Here S_n is the symmetric group of degree n .

Later we are also interested in truncated Fock space for describing situations with at most N particles,

$$\mathcal{F}_N = \bigoplus_{n=0}^N \mathcal{H}^{\otimes n} \subset \mathcal{F}, \quad (4)$$

and truncated bosonic Fock space $\mathcal{F}_N^S = P^S(\mathcal{F}_N)$.

Fermionic Fock \mathcal{F}^A space is introduced analogously, with symmetrisation P^S replaced by anti-symmetrisation P^A acting on $\phi \in \mathcal{F}$ as

$$(P^A \phi)^n(x_1, \dots, x_n) = \frac{1}{n!} \sum_{\sigma \in S_n} \text{sign}(\sigma) \phi^n(x_{\sigma(1)}, \dots, x_{\sigma(n)}). \quad (5)$$

Scalar product and norm on \mathcal{F} are induced from the scalar product on the one-particle Hilbert space \mathcal{H} , in particular for $\mathcal{H} = L^2(\mathbb{R})$ and $\phi, \psi \in \mathcal{F}$ we have

$$\langle \phi, \psi \rangle = \overline{\phi^0} \psi^0 + \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} \overline{\phi^n(x_1, \dots, x_n)} \psi^n(x_1, \dots, x_n) dx_1 \dots dx_n. \quad (6)$$

On \mathcal{F} one can define operators $a(f)$ which annihilate a particle with normalised wave function f , by

$$(a(f)\phi)^n(x_1, \dots, x_n) = \sqrt{n+1} \int_{-\infty}^{\infty} \overline{f(x)} \phi^{n+1}(x_1, \dots, x_n, x) dx \quad \forall n \geq 0. \quad (7)$$

Note that $a(f)$ leaves the bosonic and fermionic subspaces \mathcal{F}^S and \mathcal{F}^A invariant. The adjoint of $a(f)$ on \mathcal{F}^S , the bosonic creation operator $a^\dagger(f)$, acts as

$$(a^\dagger(f)\phi)^n(x_1, \dots, x_n) = \frac{1}{\sqrt{n}} \sum_{j=1}^n f(x_j) \phi^{n-1}(x_1, \dots, x_{j-1}, x_{j+1}, \dots, x_n) \quad \forall n \geq 1 \quad (8)$$

$$\text{and} \quad (a^\dagger(f)\phi)^0 = 0.$$

On \mathcal{F}^A , i.e. for fermions, one has to include an additional factor $(-1)^{j+1}$ inside the sum.

Now we would like to describe bosons which can be created and annihilated at an external source located at position y and which otherwise move freely. Free propagation is described by $-\Delta^{\mathcal{F}}$ (in units where $\hbar = 2m = 1$) which is defined as

$$(\Delta^{\mathcal{F}} \phi)^n = \sum_{j=1}^n \Delta_j \phi^n \quad (9)$$

where Δ_j denotes the second derivative with respect to the j^{th} argument. Thus, our tentative Hamiltonian reads

$$H = -\Delta^{\mathcal{F}} + \bar{c}a(\delta_y) + ca^\dagger(\delta_y), \quad (10)$$

where $\delta_y(x) = \delta(x - y)$ denotes the Dirac delta function and $c \in \mathbb{C}$ is a coupling constant. However, since δ_y is not a smooth function but a distribution, the creation operator $a^\dagger(\delta_y)$ cannot even be densely defined on \mathcal{F}^S , cf. e.g. [10, Sec. X.7], i.e. as it stands Eq. (10) does not make sense. But we can try to give meaning to Eq. (10) in the same way as δ -potentials are treated in textbook quantum mechanics. To this end we write out the eigenvalue equation $H\phi = E\phi$ in the n -particle sector ($n \geq 1$),

$$\begin{aligned} -\sum_{j=1}^n (\Delta_j \phi^n)(x_1, \dots, x_n) + \bar{c}\sqrt{n+1} \phi^{n+1}(x_1, \dots, x_n, y) \\ + \frac{c}{\sqrt{n}} \sum_{j=1}^n \delta(x_j - y) \phi^{n-1}(x_1, \dots, x_{j-1}, x_{j+1}, \dots, x_n) = E \phi^n(x_1, \dots, x_n), \end{aligned} \quad (11)$$

integrate in one variable, say x_n , from $y - \varepsilon$ to $y + \varepsilon$, and take the limit $\varepsilon \rightarrow 0+$. We obtain

$$-\left[(\partial_n \phi^n)(x_1, \dots, x_n)\right]_{x_n=y-}^{x_n=y+} + \frac{c}{\sqrt{n}} \phi^{n-1}(x_1, \dots, x_{n-1}) = 0, \quad (12)$$

where ∂_j denotes the derivative with respect to the j th argument. We have thus found a condition coupling neighbouring sectors in Fock space, which replaces the ill-defined creation operator in Eq. (10). Following Teufel and Tumulka [1, 2] we will refer to Eq. (12) as an interior-boundary condition (IBC). Rewriting Eq. (12), for $c \neq 0$ our model now reads

$$\begin{aligned} H &= -\Delta^{\mathcal{F}} + \bar{c}a(\delta_y) \\ \text{with IBC } \phi^n(x_1, \dots, x_n) &= \frac{\sqrt{n+1}}{c} \left[(\partial_{n+1} \phi^{n+1})(x_1, \dots, x_{n+1}) \right]_{x_{n+1}=y-}^{x_{n+1}=y+}. \end{aligned} \quad (13)$$

This is the one-dimensional analogue of the condition which is called Dirichlet-IBC in Ref. [1], as we demonstrate in Appendix A. In [4] it is shown that the IBC-Hamiltonian is essentially self-adjoint when defined on a suitable domain. Models with several point sources can be written down in the same way, by adding additional annihilation operators to the Hamiltonian, supplemented by the corresponding IBCs, see also Sec. IV. Inspection of the IBC in Eq. (13) reveals that ϕ^n uniquely determines $\phi^\nu \forall \nu < n$. Moreover, the IBC ensures that ϕ^n inherits the symmetry of ϕ^{n+1} , i.e. although derived for bosons, only a factor $(-1)^n$ inside the square brackets is required in order to define the corresponding IBC-Hamiltonian for fermions.

The IBC-Hamiltonian (13) is, up to a translation in energy, unitarily equivalent to the free Hamiltonian $-\Delta^{\mathcal{F}}$, a result which we will discuss elsewhere. (The analogous statement

for the 3D IBC-Hamiltonian is shown in [4, 5].) In Secs. III–V we instead focus on the truncated IBC-Hamiltonian on \mathcal{F}_1^S , i.e. we do not allow creation of more than one particle. Correspondingly, $\phi = (\phi^0, \phi^1)$ and the IBC-Hamiltonian reads

$$(H\phi)^1 = -\phi^{1''}, \quad (H\phi)^0 = \bar{c}\phi^1(0) \quad \text{with IBC} \quad \phi^0 = \frac{1}{c} \left[\phi^{1'}(x) \right]_{x=0-}^{x=0+}, \quad (14)$$

where we have, without loss of generality, also specialised to $y = 0$.

Teufel and Tumulka emphasise that for their choice of IBC (in three dimensions) probability is not conserved within Fock space sectors with fixed numbers of particles, but that it is conserved on full Fock space. In particular, the IBC enables probability flow between Fock space sectors with different numbers of particles. The same is true for the one-dimensional IBC models of Eqs. (13) and (14) which can be seen as follows. Consider, e.g., the time dependent Schrödinger equation $i\dot{\phi} = H\phi$ with Hamiltonian and IBC (14), i.e. sectorwise we have

$$i\dot{\phi}^1(x, t) = -\phi^{1''}(x, t), \quad x \neq 0 \quad \text{and} \quad (15)$$

$$i\dot{\phi}^0(t) = \bar{c}\phi^1(0, t). \quad (16)$$

From Eq. (15) one can derive the continuity equation $\dot{\rho}^1(x, t) + j^{1'}(x, t) = 0$, $x \neq 0$, in the one-particle sector, with probability density $\rho^1(x, t) = |\phi^1(x, t)|^2$ and current $j^1(x, t) = 2 \text{Im}(\overline{\phi^1(x, t)}\phi^{1'}(x, t))$ as usual. However, at $x = 0$, the position of the source, the current is generally discontinuous. According to the IBC the flow into the origin is

$$[-j^1(x, t)]_{x=0-}^{x=0+} = -2 \text{Im}(\overline{c\phi^1(0, t)}\phi^0(t)). \quad (17)$$

This is compensated by the continuity equation in the zero-particle sector,

$$\frac{d}{dt}|\phi^0(t)|^2 = -2 \text{Im}(\overline{c\phi^1(0, t)}\phi^0(t)), \quad (18)$$

which is readily derived from Eq. (16). Notice that Eqs. (17) and (18) imply that for stationary states, i.e. for solutions of the time-independent Schrödinger equation $H\phi = E\phi$, there can be no net flux between the zero-particle and the one-particle sector.

III Spectrum and (generalised) eigenfunctions for one source

We consider the eigenvalue equation $H\phi = E\phi$ for the one-dimensional IBC-Hamiltonian (14) with $x \in \mathbb{R}$. As ϕ^1 has to solve $-\phi^{1''}(x) = E\phi^1(x)$ for $x \neq 0$ we distinguish the cases of negative energy, $E < 0$, and positive energy, $E > 0$.

Ground state ($E < 0$). For negative energy we make the ansatz $\phi^1(x) = Ae^{-\kappa|x|}$ with $\kappa > 0$, which solves the eigenvalue equation in the one-particle sector with $E = -\kappa^2$. Combining the eigenvalue equation in the zero-particle sector, $E\phi^0 = \bar{c}A$, with the IBC, $\phi^0 = -2A\kappa/c$, yields the condition $2\kappa^3 = |c|^2$. Together with the normalisation condition

$$\|(\phi_g^0, \phi_g^1)\|^2 = |A|^2 \frac{4\kappa^2}{|c|^2} + |A|^2 \int_{-\infty}^{\infty} e^{-2\kappa|x|} dx = |A|^2 \left(\frac{2}{\kappa} + \frac{1}{\kappa} \right) = 1, \quad (19)$$

we find $A = \sqrt{\kappa/3}$ and obtain the normalised ground state

$$\phi_g = (\phi_g^0, \phi_g^1), \quad \phi_g^0 = -\sqrt{\frac{2}{3}} \frac{|c|}{c}, \quad \phi_g^1(x) = \sqrt{\frac{\kappa}{3}} e^{-\kappa|x|}, \quad \kappa = \sqrt[3]{\frac{|c|^2}{2}}, \quad (20)$$

with energy $E_g = -\kappa^2$. Note that the state has a weight of $2/3$ in the zero-particle sector and a weight of $1/3$ in the one-particle sector

$$\overline{\phi_g^0} \phi_g^0 = \frac{2}{3}, \quad \int_{-\infty}^{\infty} \overline{\phi_g^1(x)} \phi_g^1(x) dx = \frac{1}{3}, \quad (21)$$

with sum $\|\phi_g\|^2 = \langle \phi_g, \phi_g \rangle = 1$. In limit $c \rightarrow 0$ ϕ_g becomes proportional to the free vacuum $\phi_{\text{vac}} = (\phi_{\text{vac}}^0, \phi_{\text{vac}}^1) = (1, 0)$, but the normalisation is lost. In appendix B we show how ϕ_{vac} can be recovered from ϕ_g in the limit of vanishing coupling by first introducing a zero point energy.

In the following it is often convenient to express c in terms of κ and write $c = \sqrt{2\kappa^3} e^{i\varphi_c}$ where φ_c is the phase of c .

Scattering states (generalised eigenfunctions for $E > 0$). In the one-particle sector we make the ansatz

$$\phi_k^1(x) = \frac{1}{\sqrt{2\pi}} (e^{ikx} + b_k e^{i|k||x|}), \quad k \in \mathbb{R} \setminus \{0\}, \quad (22)$$

of a (flux normalised) plane wave plus a one-dimensional “spherical” wave. For $x \neq 0$ we have $-\Delta \phi_k^1 = k^2 \phi_k^1$, i.e. the energy of the tentative solution is $E_k = k^2$. From the IBC follows

$$\phi_k^0 = \frac{2i|k|}{\sqrt{2\pi} c} b_k, \quad (23)$$

and together with $(H\phi)^0 = E\phi^0$ we obtain

$$\frac{\bar{c}}{\sqrt{2\pi}} (1 + b_k) = E \frac{2i|k|}{\sqrt{2\pi} c} b_k \quad \Leftrightarrow \quad b_k = \frac{|c|^2}{2i|k|^3 - |c|^2} = \frac{-i\kappa^3}{|k|^3 + i\kappa^3}. \quad (24)$$

The scattering states (22), being solutions of the time-independent Schrödinger equation, conserve the probability flux within the one-particle sector, cf. the remark following Eq. (18). In the language of scattering theory, this can also be seen by decomposing ϕ_k^1 into an incoming wave, a reflected wave with reflection amplitude $r_k = b_k$, and a transmitted wave with transmission amplitude $t_k = 1 + b_k$. Then flux conservation within the one-particle sector means that reflection and transmission coefficients add to unity, $|r_k|^2 + |t_k|^2 = 1$, which is equivalent to $\text{Re } b_k = -|b_k|^2$, a condition fulfilled by (24).

Notice that $\lim_{c \rightarrow 0} b_k = 0$ as well as $\lim_{c \rightarrow 0} \phi_k^0 = 0$, i.e. for vanishing coupling the solution $\phi_k = (\phi_k^0, \phi_k^1)$ goes over to an ordinary plane wave supported only in the one-particle sector.

The scattering states (22) with coefficients b_k from (24) are very similar to those for a system with delta potential in single-particle quantum mechanics: A particle subject to a

potential $\lambda\delta(x)$, but otherwise free, has scattering states of the form (22) with b_k replaced by the reflection amplitude $\lambda/(2i|k| - \lambda)$ [11]. Hence the scattering solutions (22) formally look like those for a delta potential with (energy-dependent) parameter $\lambda = |c|^2/E$.

Ground state and scattering states form an orthonormal set satisfying

$$\langle \phi_g, \phi_g \rangle = 1, \quad \langle \phi_g, \phi_k \rangle = 0, \quad \langle \phi_{k'}, \phi_k \rangle = \delta(k - k'), \quad (25)$$

for all $k, k' \in \mathbb{R} \setminus \{0\}$. The first relation was obtained above and the other two are derived in Appendix C.

Completeness. Having established orthonormality we now move on to show that (ϕ_g^0, ϕ_g^1) and (ϕ_k^0, ϕ_k^1) form a complete set. Completeness means that any $\phi = (\phi^0, \phi^1) \in \mathcal{F}_1^S$ can be expanded as follows,

$$\phi = a_g \phi_g + \int_{-\infty}^{\infty} a_k \phi_k dk. \quad (26)$$

Due to orthonormality the expansion coefficients can be calculated by taking scalar products,

$$a_g = \langle \phi_g, \phi \rangle, \quad a_k = \langle \phi_k, \phi \rangle. \quad (27)$$

Inserting the coefficients into the expansion, Eq. (26) becomes, sectorwise,

$$\begin{aligned} \phi^0 &= \left(|\phi_g^0|^2 + \int_{-\infty}^{\infty} |\phi_k^0|^2 dk \right) \phi^0 + \int_{-\infty}^{\infty} \left(\overline{\phi_g^1(y)} \phi_g^0 + \int_{-\infty}^{\infty} \overline{\phi_k^1(y)} \phi_k^0 dk \right) \phi^1(y) dy, \\ \phi^1(x) &= \left(\overline{\phi_g^0} \phi_g^1(x) + \int_{-\infty}^{\infty} \overline{\phi_k^0} \phi_k^1(x) dk \right) \phi^0 \\ &\quad + \int_{-\infty}^{\infty} \left(\overline{\phi_g^1(y)} \phi_g^1(x) + \int_{-\infty}^{\infty} \overline{\phi_k^1(y)} \phi_k^1(x) dk \right) \phi^1(y) dy. \end{aligned} \quad (28)$$

These equations hold for every ϕ if and only if

- (i) $|\phi_g^0|^2 + \int_{-\infty}^{\infty} |\phi_k^0|^2 dk = 1,$
- (ii) $\overline{\phi_g^0} \phi_g^1(x) + \int_{-\infty}^{\infty} \overline{\phi_k^0} \phi_k^1(x) dk = 0 \quad \text{and}$
- (iii) $\overline{\phi_g^1(y)} \phi_g^1(x) + \int_{-\infty}^{\infty} \overline{\phi_k^1(y)} \phi_k^1(x) dk = \delta(x - y).$

These three relations are shown to hold for the solutions ϕ_g and ϕ_k in Appendix C.

Green function. The resolvent $(E - H)^{-1}$ of the IBC-Hamiltonian on \mathcal{F}_1^S has the spectral decomposition

$$\frac{1}{E - H} = \frac{\langle \phi_g, \cdot \rangle \phi_g}{E - E_g} + \int_{-\infty}^{\infty} \frac{\langle \phi_k, \cdot \rangle \phi_k}{E - E_k} dk. \quad (29)$$

If we express the resolvent in the position representation then we obtain the Green function. Letting $(E - H)$ act on the Green function one obtains from (14) and (29) the following equations in the different sectors

$$\begin{aligned} \left(E + \frac{d^2}{dx^2}\right) G^{11}(x, y, E) &= \delta(x - y), & E G^{01}(y, E) - \bar{c} G^{11}(0, y, E) &= 0, \\ \left(E + \frac{d^2}{dx^2}\right) G^{10}(x, E) &= 0, & E G^{00}(E) - \bar{c} G^{10}(0, E) &= 1, \end{aligned} \quad (30)$$

for $x \neq 0$. They are subject to the IBCs

$$\begin{aligned} G^{01}(y, E) &= \frac{1}{c} \left[\frac{d}{dx} G^{11}(x, y, E) \right]_{x=0-}^{x=0+}, & G^{00}(E) &= \frac{1}{\bar{c}} \left[\frac{d}{dy} G^{01}(y, E) \right]_{y=0-}^{y=0+}, \\ G^{10}(x, E) &= \frac{1}{\bar{c}} \left[\frac{d}{dy} G^{11}(x, y, E) \right]_{y=0-}^{y=0+}, & G^{00}(E) &= \frac{1}{c} \left[\frac{d}{dx} G^{10}(x, E) \right]_{x=0-}^{x=0+}. \end{aligned} \quad (31)$$

The solutions to (30) and (31) can be obtained directly from the scattering states (22). Let $k = \sqrt{E} > 0$. Then the (retarded) Green function is given in the 11-sector by

$$G^{11}(x, y, E) = \frac{\phi_{-k}^1(x_{<}) \phi_k^1(x_{>})}{W(y)}, \quad (32)$$

where $x_{>}$ ($x_{<}$) is the larger (smaller) of x and y , and $W(y) = \phi_{-k}^1(y) \phi_k^{1'}(y) - \phi_k^1(y) \phi_{-k}^{1'}(y)$ is the Wronskian. Formulas of the form (32) are used in Sturm-Liouville theory, see e.g. [12, Sec. 7.2]. The term $\phi_{-k}^1(x_{<})$ has the correct outgoing behaviour as $x \rightarrow -\infty$, whereas $\phi_k^1(x_{>})$ is outgoing for $x \rightarrow \infty$. With (22) we obtain $W = 2ik(1 + b_k)$, and from (32)

$$G^{11}(x, y, E) = \frac{1}{2ik} e^{ik|x-y|} + \frac{b_k}{2ik} e^{ik|x|} e^{ik|y|}. \quad (33)$$

Again this has a similar form as for a delta potential $\lambda\delta(x)$, see [11]. As before, the difference is that $|c|^2/E$ replaces λ . The Green function in the other sectors follows from (31),

$$G^{01}(y, E) = \frac{b_k}{c} e^{ik|y|}, \quad G^{10}(x, E) = \frac{b_k}{\bar{c}} e^{ik|x|}, \quad G^{00}(E) = \frac{2ikb_k}{|c|^2}. \quad (34)$$

It can easily be checked that these solutions satisfy the relations (30). For negative energies one has to set $k = i\sqrt{-E}$.

In order to develop an intuitive interpretation of the Green function, we define a diffraction coefficient $\mathcal{D} = 2ikb_k$ which allows us to rewrite Eq. (33) as

$$G^{11}(x, y, E) = G_0(x, y, E) + G_0(x, 0, E) \mathcal{D} G_0(0, y, E). \quad (35)$$

Here $G_0(x, y, E) = \exp(ik|x-y|)/2ik$ is the free single-particle Green function in one dimension. In the semiclassical limit $k \rightarrow \infty$ the Green function can be interpreted in terms

of particle trajectories, and in the case at hand the semiclassical approximation coincides with the exact Green function. In (35) there is a contribution from a direct path from y to x , and a second path from y to the origin where it is diffracted due to the interaction with the vacuum and then continues to x . This agrees with the general form expected according to Keller's geometrical theory of diffraction [13, 14]. Since for the IBC-Hamiltonian the only interactions possible at the origin are particle creation and annihilation, we would like to interpret \mathcal{D} as the amplitude for annihilation and subsequent re-creation of a particle. Consequently, G^{11} displays flux conservation in the one-particle sector. For Green functions this is expressed by the optical theorem which here takes the form $\text{Im } \mathcal{D} = -|\mathcal{D}|^2/2k$, cf. [15].

Before we can interpret the Green function in all sectors in terms of particle creation and annihilation we need to introduce one more notion. In the same way as we refer to $G_0(x, y, E)$ as the amplitude for a particle going from y to x along a straight line, let us call $G^{00}(E)$ the amplitude for staying in the vacuum. Now we can once more rewrite the Green function,

$$\begin{aligned} G^{11}(x, y, E) &= G_0(x, y, E) + G_0(x, 0, E) c G^{00}(E) \bar{c} G_0(0, y, E) \\ G^{01}(y, E) &= G^{00}(E) \bar{c} G_0(0, y, E), \\ G^{10}(x, E) &= G_0(x, 0, E) c G^{00}(E). \end{aligned} \tag{36}$$

Recall that according to the IBC-Hamiltonian particle creation is associated with a factor c , whereas particle annihilation is associated with a factor \bar{c} . This is made most obvious in the naive Hamiltonian (10). Now all components of the Green function can be interpreted in the same way. $G^{01}(y, E)$ is the amplitude for a particle going from y to the origin where it is annihilated, and then the system stays in the vacuum. The reverse process is described by $G^{10}(x, E)$, with the system starting in the vacuum, then a particle is created and moves to x . Finally, the diffractive contribution to $G^{11}(x, y, E)$ can be interpreted as the amplitude for a particle going from y to the origin where it is annihilated, intermediately leaving the system in the vacuum, and then the particle is re-created and moves to x .

Time evolution. Stationary solutions at constant energy E cannot have a net probability flux between the zero-particle and the one-particle sector. The situation is different for the time evolution of general states. Consider a state $\phi(t)$ satisfying the initial condition $\phi(0) = \phi_0 \in \mathcal{F}_1^S$. For times $t > 0$ it can be expressed in the two sectors in terms of the initial state $\phi_0 = (\phi_0^0, \phi_0^1)$ and the kernel K of the time evolution operator,

$$\begin{aligned} \phi^1(x, t) &= \int_{-\infty}^{\infty} K^{11}(x, y, t) \phi_0^1(y) dy + K^{10}(x, t) \phi_0^0, \\ \phi^0(t) &= \int_{-\infty}^{\infty} K^{01}(y, t) \phi_0^1(y) dy + K^{00}(t) \phi_0^0. \end{aligned} \tag{37}$$

The time evolution kernel for the IBC-Hamiltonian (14) is derived in appendix D and given explicitly in Eqs. (134) and (136). We consider here only one example. Assume that the

initial state is the free vacuum $\phi_0 = \phi_{\text{vac}} = (\phi_{\text{vac}}^0, \phi_{\text{vac}}^1) = (1, 0)$. For $t > 0$ it evolves to

$$\phi^1(x, t) = K^{10}(x, t), \quad \phi^0(t) = K^{00}(t). \quad (38)$$

At initial time $t = 0$ the state has weight 1 in the zero-particle sector. Then an interesting question is how the weight changes as $t \rightarrow \infty$. This follows from the asymptotics of $K^{00}(t)$ as $t \rightarrow \infty$ which is evaluated in (138),

$$\phi^0(t) = K^{00}(t) \sim \frac{2}{3} e^{i\kappa^2 t} + \mathcal{O}(t^{-3/2}) \quad \text{as } t \rightarrow \infty. \quad (39)$$

Hence the weight in the zero-particle sector decreases from 1 to $4/9$ as $t \rightarrow \infty$.

IV Several sources

In this section, we first consider the case of two sources on the real line. We are particularly interested in the ground state energy and its dependence on the distance of the sources. Placing the sources at $y_1 = 0$ and $y_2 = R$, the model reads

$$\begin{aligned} (H\phi)^1 &= -\phi^{1''}, & (H\phi)^0 &= \bar{c}_1 \phi^1(0) + \bar{c}_2 \phi^1(R) \\ \text{with IBCs} \quad \phi^0 &= \frac{1}{c_1} \left[\phi^{1'}(x) \right]_{x=0-}^{x=0+}, & \phi^0 &= \frac{1}{c_2} \left[\phi^{1'}(x) \right]_{x=R-}^{x=R+}, \end{aligned} \quad (40)$$

and with coupling constants c_1 and c_2 . Thinking of the sources as particles of a different kind pinned at a distance R , the constants c_1 and c_2 represent the charges, with which these pinned particles couple to the dynamical particles of our model. Hence, the dependence of the ground state energy on the distance of the sources should be interpreted as the potential between the charges generated by the exchange of particles in \mathcal{F}_1^S .

Ground state. As we are interested in the ground state energy we search for solutions to $H\phi = E\phi$ with negative energy $E < 0$. Away from the sources, ϕ^1 has to satisfy $-\phi^{1''} = E\phi^1$, and the most general ansatz for a continuous normalisable solution with negative energy and discontinuous derivatives at $x = 0$ and $x = R$ is

$$\phi^1(x) = a e^{-\kappa|x|} + b e^{-\kappa|x-R|}, \quad \kappa > 0, \quad E = -\kappa^2. \quad (41)$$

The IBCs allow to express the coefficients a and b in terms of the zero-particle sector wave function ϕ^0 ,

$$a = -\frac{c_1}{2\kappa} \phi^0, \quad b = -\frac{c_2}{2\kappa} \phi^0. \quad (42)$$

Then the eigenvalue equation in the zero-particle sector reads

$$-\left(\frac{|c_1|^2 + |c_2|^2}{2\kappa} + \frac{\bar{c}_1 c_2 + \bar{c}_2 c_1}{2\kappa} e^{-\kappa|R|} \right) \phi^0 = E\phi^0. \quad (43)$$

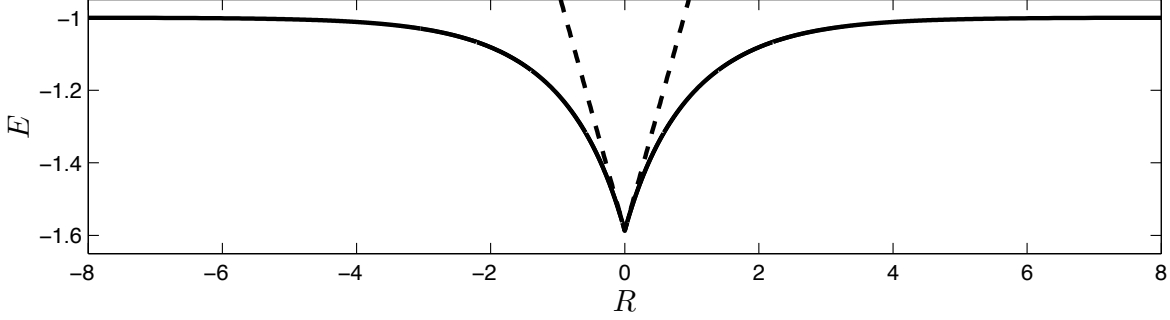


Figure 1: Ground state energy for two sources with coupling constants $c_1 = c_2 = 1$ and separation R . The dashed lines show the linear approximation (45).

This defines the ground state energy $E(R)$ as a function of the distance of the two sources. Substituting $\kappa = \sqrt{-E}$ we first observe that

$$E(0) = - \left(\frac{|c_1 + c_2|^2}{2} \right)^{2/3} \quad \text{and} \quad \lim_{|R| \rightarrow \infty} E(R) = - \left(\frac{|c_1|^2 + |c_2|^2}{2} \right)^{2/3}. \quad (44)$$

For small $|R|$ we can expand the exponential in Eq. (43) and find the linear approximation

$$E(R) \sim - \left(\frac{|c_1 + c_2|^2}{2} \right)^{2/3} + \frac{\bar{c}_1 c_2 + \bar{c}_2 c_1}{3} |R|, \quad |R| \rightarrow 0, \quad (45)$$

i.e. for small distances the ground state energy behaves like a one-dimensional Coulomb potential. With real charges c_1 and c_2 the potential is attractive if the charges have the same sign, and repulsive for opposite signs, which is to be expected for a scalar field. In Fig. 1 we display $E(R)$ for $c_1 = c_2 = 1$ along with the approximation for small $|R|$ (dashed line).

Scattering states. For the scattering states we make the ansatz

$$\phi_k^1(x) = \frac{1}{\sqrt{2\pi}} \left(e^{ikx} + b_k e^{i|k||x|} + \tilde{b}_k e^{i|k||x-R|} \right), \quad k \in \mathbb{R} \setminus \{0\}. \quad (46)$$

These functions satisfy $-\phi_k^{1''} = k^2 \phi_k^1$ for $x \notin \{0, R\}$ and have energy $E_k = k^2$. From the IBCs follows

$$\phi_k^0 = \frac{2i|k| b_k}{\sqrt{2\pi} c_1} \quad \text{and} \quad \phi_k^0 = \frac{2i|k| \tilde{b}_k}{\sqrt{2\pi} c_2}, \quad (47)$$

and from $(H\phi)^0 = E\phi^0$ we obtain

$$E\phi_k^0 = \frac{\bar{c}_1}{\sqrt{2\pi}} \left(1 + b_k + \tilde{b}_k e^{i|k||R|} \right) + \frac{\bar{c}_2}{\sqrt{2\pi}} \left(e^{ikR} + b_k e^{i|k||R|} + \tilde{b}_k \right). \quad (48)$$

Inserting (47) we find

$$\phi_k^0 = \frac{2i|k| (\bar{c}_1 + \bar{c}_2 e^{ikR})}{\sqrt{2\pi} (2i|k|^3 - |c_1|^2 - |c_2|^2 - (c_1 \bar{c}_2 + \bar{c}_1 c_2) e^{i|k||R|})}, \quad (49)$$

and b_k and \tilde{b}_k follow from (47). In the case of just one source we were able to map (generalised) eigenfunctions to solutions of a single-particle Schrödinger equation with delta scatterer, see Sec. III. For two sources it is no longer possible to map the amplitudes b_k and \tilde{b}_k to the corresponding amplitudes for two delta scatterers in single-particle quantum mechanics. The reason for this is that the two sources do not act as independent scatterers but are connected by the vacuum.

More than two sources. The results of this section can easily be generalised to several sources. Then one has

$$(H\phi)^1 = -\phi^{1''}, \quad (H\phi)^0 = \sum_{i=1}^n \bar{c}_i \phi^1(x_i), \quad \phi^0 = \frac{1}{c_i} \left[\phi^{1'}(x) \right]_{x=x_i-}^{x=x_i+}, \quad i = 1, \dots, n, \quad (50)$$

for n sources with coupling constants c_i at positions x_i . The ground state has the form

$$\phi_g^1(x) = \sum_{i=1}^n a_i e^{-\kappa|x-x_i|}, \quad \kappa > 0, \quad E = -\kappa^2, \quad (51)$$

from the IBCs one obtains

$$a_i = -\frac{c_i}{2\kappa} \phi_g^0, \quad i = 1, \dots, n, \quad (52)$$

and the energy $E = -\kappa^2$ follows from the eigenvalue equation in the zero-particle sector

$$2\kappa^3 = \sum_{i,j=1}^n \bar{c}_i c_j e^{-\kappa|x_i-x_j|}. \quad (53)$$

The scattering states have the form

$$\phi_k^1(x) = \frac{1}{\sqrt{2\pi}} \left(e^{ikx} + \sum_{i=1}^n b_i e^{i|k||x-x_i|} \right), \quad k \in \mathbb{R} \setminus \{0\}, \quad E = k^2, \quad (54)$$

from the IBCs one obtains

$$b_i = \sqrt{2\pi} \frac{c_i}{2i|k|} \phi_k^0, \quad i = 1, \dots, n, \quad (55)$$

and from the eigenvalue equation in the zero-particle sector follows

$$\phi_k^0 = \frac{2i|k| \sum_{i=1}^n \bar{c}_i e^{ikx_i}}{\sqrt{2\pi} \left(2i|k|^3 - \sum_{i,j=1}^n \bar{c}_i c_j e^{i|k||x_i-x_j|} \right)}. \quad (56)$$

V Particle in a box with one source

An example of a system with a discrete spectrum is a particle in a box of length l with one source. We place the source at $x = 0$ and require Dirichlet boundary conditions at the end points $x = -l_1 < 0$ and $x = l_2 > 0$ where $l_1 + l_2 = l$.

Negative energies. The general ansatz for an eigenfunction with energy $E = -\kappa^2$, $\kappa > 0$, which satisfies Dirichlet conditions at $-l_1$ and l_2 is

$$\phi^1(x) = \begin{cases} A \sinh(\kappa(x + l_1)), & x < 0, \\ B \sinh(\kappa(x - l_2)), & x > 0. \end{cases} \quad (57)$$

Continuity at $x = 0$ requires

$$A \sinh(\kappa l_1) = -B \sinh(\kappa l_2). \quad (58)$$

The IBC (14) determines the zero-particle sector wave function,

$$\phi^0 = \frac{\kappa}{c} (B \cosh(\kappa l_2) - A \cosh(\kappa l_1)), \quad (59)$$

and together with $(H\phi)^0 = \bar{c}A \sinh(\kappa l_1)$ the eigenvalue equation demands

$$|c|^2 A \sinh(\kappa l_1) = -\kappa^3 (B \cosh(\kappa l_2) - A \cosh(\kappa l_1)), \quad (60)$$

which, using (58), can be expressed as

$$\kappa^3 = |c|^2 \frac{\sinh(\kappa l_1) \sinh(\kappa l_2)}{\sinh(\kappa l)}. \quad (61)$$

This equation has exactly one positive solution κ for any $l_1, l_2 > 0$. This can be seen by considering the left- and right-hand sides of (61) as functions of $\kappa \geq 0$. Both functions start at zero. The left-hand side has a slope that is monotonously increasing from zero to infinity. The function on the right-hand side has a slope that is positive and monotonously decreasing, as we show below. Hence the two functions intersect exactly once.

To prove the statement about the derivative of the right-hand side consider

$$\frac{d}{d\kappa} \frac{\sinh(\kappa l_1) \sinh(\kappa l_2)}{\sinh(\kappa l)} = \frac{l_1 \sinh^2(\kappa l_2) + l_2 \sinh^2(\kappa l_1)}{\sinh^2(\kappa l)}. \quad (62)$$

This is positive for $\kappa \geq 0$. It is also monotonously decreasing because $\sinh(\kappa l_2)/\sinh(\kappa l)$ and $\sinh(\kappa l_1)/\sinh(\kappa l)$ are monotonously decreasing. This follows, for example, from

$$\frac{d}{d\kappa} \frac{\sinh(\kappa l_1)}{\sinh(\kappa l)} = \frac{l_1 \sinh(\kappa l_2) - l_2 \sinh(\kappa l_1) \cosh(\kappa l)}{\sinh^2(\kappa l)} < \frac{l_1 \sinh(\kappa l_2) - \kappa l_1 l_2 \cosh(\kappa l_2)}{\sinh^2(\kappa l)} < 0, \quad (63)$$

where the last inequality holds since $\sinh(z) - z \cosh(z) < 0 \forall z > 0$.

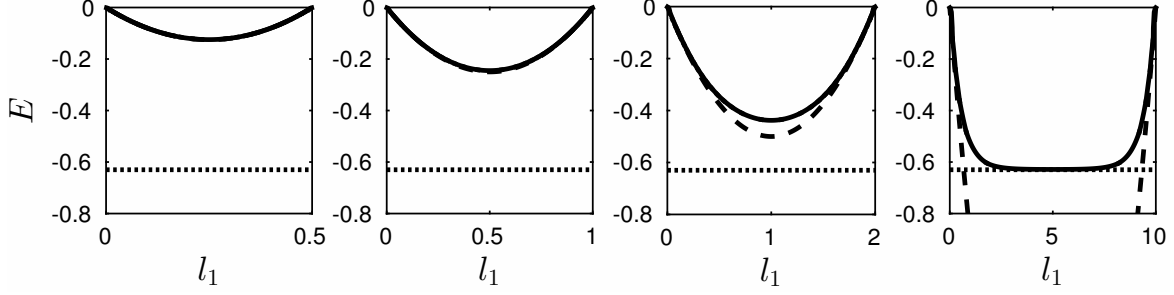


Figure 2: Ground state energy for coupling $|c| = 1$ determined by Eq. (61) as a function of the position l_1 of the source for box lengths $l = \frac{1}{2}, 1, 2, 10$ (left to right) along with the approximation for small boxes (dashed line, almost indistinguishable from the solid line in the first two panels) and the limiting value $-2^{-2/3}$ for large boxes (dotted line).

In the limit of small boxes, $l \rightarrow 0$ with l_1/l and l_2/l constant, we find from (61) that $\kappa \sim \sqrt{|c|^2 l_1 l_2 / l}$, i.e. the energy approaches zero from below. For large boxes, $l \rightarrow \infty$ with l_1/l and l_2/l constant, we obtain $\kappa \rightarrow \kappa_0 = \sqrt[3]{|c|^2 / 2}$. This limiting value corresponds to the ground state of the IBC-Hamiltonian in Sec. III. In Fig. 2 we show the ground state energy as a function of l_1 , the relative position of the source inside the box ($0 \leq l_1 \leq l$), for different box sizes and fixed coupling. We observe an effective repulsion of the source from the boundaries, generated by emission, reflection and re-absorption of particles.

Zero energy. The general ansatz for an eigenfunction with $E = 0$ that satisfies the Dirichlet boundary conditions is

$$\phi^1(x) = \begin{cases} A(x + l_1), & x < 0 \\ B(x - l_2), & x > 0 \end{cases}. \quad (64)$$

The eigenvalue equation in the zero-particle sector then requires $A = B = 0$, and hence $E = 0$ is not an eigenvalue of the Hamiltonian.

Positive energies. For eigenfunction with energy $E = k^2$, $k > 0$, the ansatz (57) is replaced by

$$\phi^1(x) = \begin{cases} A \sin(k(x + l_1)), & x < 0, \\ B \sin(k(x - l_2)), & x > 0. \end{cases} \quad (65)$$

A similar calculation as before then leads to the eigenvalue condition

$$-k^3 = |c|^2 \frac{\sin(kl_1) \sin(kl_2)}{\sin(kl)}. \quad (66)$$

In the following we derive spectral determinant and trace formula for the particle in a box with IBC. We start by first considering a particle in a box without IBCs.

Green function for box without source. The Green function is obtained from the general formula (32) by choosing for the left and right functions $\sin(k(x_{<} + l_1))$ and $\sin(k(x_{>} - l_2))$. These are solutions of the Schrödinger equation that satisfy the left and

right Dirichlet boundary condition, respectively. With the Wronskian $W(y) = k \sin(kl)$ we obtain

$$G_b(x, y, E) = \frac{\sin(k(x_{<} + l_1)) \sin(k(x_{>} - l_2))}{k \sin(kl)}. \quad (67)$$

From the poles one reads off the eigenvalue condition $\sin(kl) = 0$, $k \neq 0$. Note that (67) can also be obtained by applying mirror images to satisfies the boundary conditions

$$G_b(x, y, E) = \sum_{n=-\infty}^{\infty} G_0(x, y + 2nl, E) - \sum_{n=-\infty}^{\infty} G_0(x, -y - 2l_1 + 2nl, E), \quad (68)$$

where G_0 is the free Green function (after (35)). As discussed earlier, G_0 coincides with its semiclassical approximation in terms of a trajectory from initial to final point. The form (68) can then be interpreted as sum over all trajectories in the box from y to x (unfolded onto the real line by the mirror principle). This agrees with the general semiclassical form of Green functions, see e.g. [16, 17].

The trace of the Green function is

$$\text{Tr } G_b(E) = \int_{-l_1}^{l_2} G_b(x, x, E) dx = \frac{l \cot(kl)}{2k} - \frac{1}{2k^2}, \quad (69)$$

from which we obtain the spectral determinant

$$\Delta_b(E) = \prod_{n=1}^{\infty} \left(1 - \frac{E}{E_n^b}\right) = \lim_{\varepsilon \rightarrow 0} \exp \left(\int_0^E \text{Tr } G_b(E + i\varepsilon) dE \right) = \frac{\sin(kl)}{kl}. \quad (70)$$

This is an entire function of $E = k^2$ with zeros at the energy levels $E_n^b = (n\pi/l)^2$, $n \in \mathbb{N}$. The spectral staircase $N(E)$ can be obtained from the spectral determinant by

$$N(E) = \sum_{n=1}^{\infty} \Theta(E - E_n) = -\frac{1}{\pi} \lim_{\varepsilon \rightarrow 0} \text{Im} \log \Delta(E + i\varepsilon) + N(0), \quad (71)$$

where Θ is the Heaviside theta function. Inserting (70) leads to

$$N_b(E) = -\frac{1}{\pi} \text{Im} \log \left[\frac{i}{2} e^{-ikl} (1 - e^{2ikl}) \right] = \frac{kl}{\pi} - \frac{1}{2} + \sum_{n=1}^{\infty} \frac{1}{\pi n} \sin(2nkl), \quad (72)$$

where we have used an expansion of $\log(1 - z)$. The result is an exact trace formula for the spectral staircase. The first two terms in the final expression are the Weyl terms for the mean staircase $\bar{N}_b(E)$, consisting of a leading order volume term and a boundary correction due to the Dirichlet boundary conditions. The oscillatory term is a sum over the periodic orbits (the orbit of length $2l$ and its repetitions)¹. A corresponding trace formula for the density of states can be obtained by differentiating (72) with respect to E .

¹Instead of adding $N(0)$ in (71) (if unknown) one can add a constant that is determined by the condition that the constant term in the asymptotic expansion of $\bar{N}(E)$ as $E \rightarrow \infty$ agrees with the coefficient of $1/E$ in the asymptotic expansion of $\text{Tr } G(E)$.

Green function for box with source. We follow the same steps for the system with IBC. The Green function is again obtained from (32). We choose as left and right functions linear combinations of the generalised eigenfunctions (22) ϕ_k and ϕ_{-k} , $k > 0$, that satisfy the left and right boundary conditions, respectively. Using the computer algebra system Maple we find

$$G^{11}(x, y, E) = G_b(x, y, E) + G_b(x, 0, E) \frac{|c|^2}{E - |c|^2 G_b(0, 0, E)} G_b(0, y, E). \quad (73)$$

This again agrees with the result for a delta potential after the replacement $|c|^2/E = \lambda$ [18]. It has also a direct semiclassical interpretation that can be seen after splitting the zero length contribution from $G_b(0, 0, E)$ by defining $G_b^- = G_b - G_0$. One then finds

$$\frac{|c|^2}{E - |c|^2 G_b(0, 0, E)} = \frac{\mathcal{D}}{1 - \mathcal{D} G_b^-(0, 0, E)} = \sum_{n=0}^{\infty} (\mathcal{D} G_b^-(0, 0, E))^n \mathcal{D}, \quad (74)$$

where $\mathcal{D} = 2ikb_k$ is the diffraction coefficient, cf. Eq. (35). After inserting (74) into (73) G^{11} can be interpreted as sum over all regular trajectories from y to x , plus a sum over all diffractive trajectories from y to x that are diffracted at the source an arbitrary number of times.

The trace of the resolvent requires also the component in the vacuum sector. It can be obtained by applying the IBCs (31),

$$G^{00}(E) = \frac{1}{E - |c|^2 G_b(0, 0, E)}. \quad (75)$$

The trace of the resolvent is evaluated using the resolvent identity,

$$\int_{-l_1}^{l_2} G_b(x, z, E) G_b(z, y, E) dz = -\frac{d}{dE} G_b(z, y, E), \quad (76)$$

leading to

$$\begin{aligned} \text{Tr } G(E) &= \int_{-l_1}^{l_2} G^{11}(x, x, E) dx + G^{00}(E) \\ &= \text{Tr } G_b(E) - \frac{|c|^2 \frac{d}{dE} G_b(0, 0, E)}{E - |c|^2 G_b(0, 0, E)} + \frac{1}{E - |c|^2 G_b(0, 0, E)} \\ &= \text{Tr } G_b(E) + \frac{d}{dE} \log(E - |c|^2 G_b(0, 0, E)). \end{aligned} \quad (77)$$

The spectral determinant follows immediately,

$$\Delta(E) = \prod_{n=1}^{\infty} \left(1 - \frac{E}{E_n}\right) = \lim_{\varepsilon \rightarrow 0} e^{\int_0^E \text{Tr } G(E+i\varepsilon) dE} = \Delta_b(E) (E - |c|^2 G_b(0, 0, E)) \frac{l}{|c|^2 l_1 l_2}. \quad (78)$$

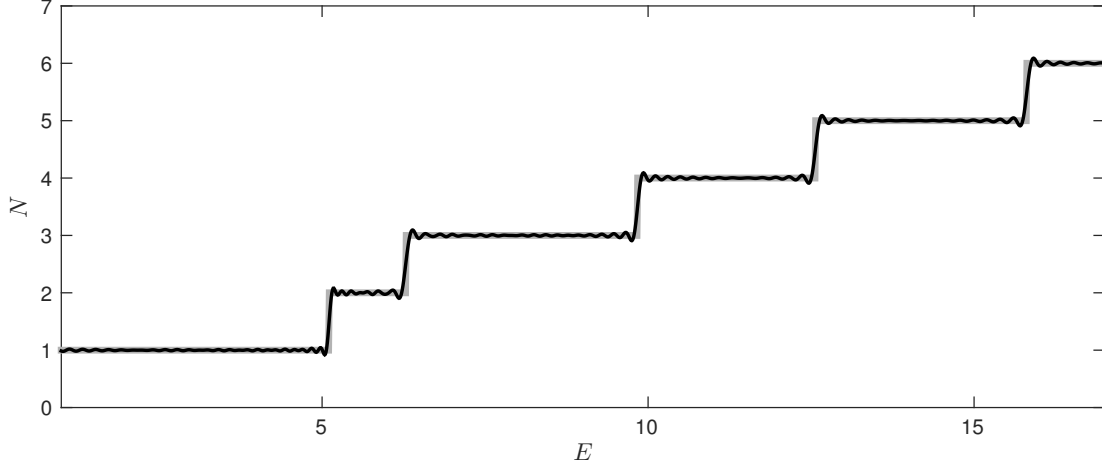


Figure 3: Spectral staircase for a box of length $l = 1$ with source in the middle, i.e. $l_1 = l_2 = \frac{1}{2}$, and coupling constant $c = 20$. We compare the exact staircase (grey) to the trace formula (81) evaluated using the 2855 shortest orbits (black).

One can check that the zeros of $\Delta(E)$ coincide with the solutions of the eigenvalue equations (61) and (66). The role of Δ_b is to cancel the poles of G_b and make the function $\Delta(E)$ entire.

In a last step we calculate the spectral staircase $N(E)$ by applying (71). With the relation

$$E - |c|^2 G_b(0, 0, E) = (E - |c|^2 G_0(0, 0, E)) (1 - \mathcal{D}G_b^-(0, 0, E)), \quad (79)$$

one obtains

$$N(E) = \frac{kl}{\pi} + \frac{1}{\pi} \arctan\left(\frac{k^3}{\kappa^3}\right) + \sum_{n=1}^{\infty} \frac{1}{\pi n} \sin(2nkl) + \sum_{n=1}^{\infty} \frac{1}{\pi n} \text{Im}(\mathcal{D}G_b^-(0, 0, E))^n \quad (80)$$

This is an exact trace formula for the spectral staircase. The source contributes a term $1/2 + \arctan(k^3/\kappa^3)/\pi$ to the mean spectral staircase plus a sum over all diffractive orbits of the system. These are closed orbits that are diffracted at the source an arbitrary number of times. Their contribution in (80) is of the general form that is expected from the geometrical theory of diffraction [14, 19, 20, 21, 22]. The diffractive orbits have the role to cancel the steps that are produced by the periodic orbits at the energy levels of the box without source, and produce new steps at the energy levels of the box with source.

The contributions of periodic and diffractive orbits can be combined and simplified by combining the term (79) with $\Delta_b(E)$ before the expansion into orbits. One then obtains

$$\begin{aligned} N(E) &= \frac{kl}{\pi} + \frac{1}{\pi} \arctan\left(\frac{k^3}{\kappa^3}\right) + \text{Im} \sum_{n=1}^{\infty} \frac{(-1)^n}{\pi n} \left(e^{2ikl + 2i \arctan(k^3/\kappa^3)} + b_k e^{2ikl_1} + b_k e^{2ikl_2} \right)^n \\ &= \frac{kl}{\pi} + \frac{1}{\pi} \arctan\left(\frac{k^3}{\kappa^3}\right) + \text{Im} \sum_{n_0, n_1, n_2=0}^{\infty} \frac{(-1)^n}{\pi n} \frac{n! b_k^{n_1+n_2}}{n_0! n_1! n_2!} e^{2ikL + 2in_0 \arctan(k^3/\kappa^3)}, \end{aligned} \quad (81)$$

where on the second line $n = n_0 + n_1 + n_2$, $L = n_0 l + n_1 l_1 + n_2 l_2$, and the prime indicates the omission of the term with $n_0 = n_1 = n_2 = 0$. Also recall that b_k is defined in (24). A numerical evaluation of the trace formula for a finite number of orbits is compared to the exact spectral staircase in Fig. 3.

VI IBCs for quantum graphs

Following the seminal work of Kottos and Smilansky [23, 24] quantum graphs have become paradigmatic in the study of quantum chaos and related areas; for overviews see e.g. [9, 25]. In this context one mainly investigates single-particle quantum mechanics on graphs. The dynamics of a fixed number of particles interacting by two-particle interactions was studied in [26, 27] for star graphs and in [28, 29, 30] for general graphs. The Fock space over a quantum graph was introduced for star graphs in [31, 32] and studied for general graphs in [33]. For some classes of graphs not only boson and fermion but also anyon statistics are possible [34, 35]; the latter we do not discuss here. In this section we demonstrate that particle creation and annihilation on Fock space over a graph can be implemented in terms of IBCs. We discuss three variants of IBCs for quantum graphs along with their different physical interpretations.

Consider a topological graph Γ consisting of N_v vertices, partially or completely connected by N_e edges. In order to simplify the notation we restrict the discussion to simple graphs, i.e. each edge connects two different vertices and no two edges connect the same two vertices. We set $a_{jk} = 1$ if the vertices j and k are connected by an edge, otherwise $a_{jk} = 0$. The (symmetric) $N_v \times N_v$ -matrix $A = (a_{jk})$ is the graph's adjacency matrix. In the following we label each edge by the pair of vertices which it connects, e.g. (jk) , $j, k \in 1, \dots, N_v$, denotes the edge connecting vertices j and k . The graph Γ becomes a metric graph by assigning a length to each edge. We denote the length of edge (jk) by $l_{(jk)}$, and consequently $l_{(jk)} = l_{(kj)}$.

The one-particle Hilbert space is a direct sum of L^2 -spaces over the edges,

$$\mathcal{H} = \bigoplus_{\substack{j,k=1 \\ k>j, a_{jk}=1}}^{N_v} L^2([0, l_{(jk)}]) \quad (82)$$

and the wave function in the n -particle sector reads

$$\phi_{(j_1 k_1) \dots (j_n k_n)}^n(x_1, \dots, x_n), \quad (83)$$

where $x_\nu \in [0, l_{(j_\nu k_\nu)}]$ is a coordinate on edge $(j_\nu k_\nu)$ which is zero at the vertex j_ν . It is convenient to also introduce an alternative coordinate on the same edge, which is zero at the vertex k_ν . This is easily accommodated within our notation by

$$\phi_{(j_\nu k_\nu) \dots}^n(\dots, x_\nu, \dots) = \phi_{(k_\nu j_\nu) \dots}^n(\dots, l_{(j_\nu k_\nu)} - x_\nu, \dots). \quad (84)$$

Wave functions are symmetrised by simultaneously permuting both, edge labels and coordinates,

$$(P^S \phi)_{(j_1 k_1) \dots (j_n k_n)}^n(x_1, \dots, x_n) = \frac{1}{n!} \sum_{\sigma \in S_n} \phi_{(j_{\sigma(1)} k_{\sigma(1)}) \dots (j_{\sigma(n)} k_{\sigma(n)})}^n(x_{\sigma(1)}, \dots, x_{\sigma(n)}). \quad (85)$$

The Laplacian $\Delta^{\mathcal{F}}$ is the edgewise second derivative

$$(\Delta^{\mathcal{F}} \phi)^n = \sum_{j=1}^n \Delta_j \phi^n. \quad (86)$$

We now want to allow particle creation and annihilation at external sources. Without loss of generality we only consider sources in vertices, since sources on edges can easily be accommodated in this scheme by cutting an edge and adding an additional vertex with valency two at this position. Hence, as Hamiltonian we choose

$$H = -\Delta^{\mathcal{F}} + \sum_{j=1}^{N_v} \bar{c}_j a(\delta_j), \quad (87)$$

where in analogy to Eqs. (7) and (10) the annihilator $a(\delta_j)$ annihilates a particle at vertex j ,

$$(a(\delta_j) \phi)_{(j_1 k_1) \dots (j_n k_n)}^n(x_1, \dots, x_n) = \frac{\sqrt{n+1}}{d_j} \sum_{k \in \Gamma_j} \phi_{(j_1 k_1) \dots (j_n k_n)(jk)}^{n+1}(x_1, \dots, x_n, 0). \quad (88)$$

Here the neighbourhood

$$\Gamma_j = \{k \mid a_{jk} = 1\} \quad (89)$$

is the set of all vertices which are connected to vertex j , and $d_j = |\Gamma_j|$ is the valency of the vertex. In each vertex, i.e. $\forall j = 1, \dots, N_v$, we demand continuity of the wave function, i.e.

$$\phi_{(jk) \dots}^n(0, \dots) = \phi_{(j\ell) \dots}^n(0, \dots) \quad \forall k, \ell \in \Gamma_j. \quad (90)$$

In analogy to Eq. (13) the IBCs read

$$\phi_{(j_1 k_1) \dots (j_n k_n)}^n(x_1, \dots, x_n) = \frac{\sqrt{n+1}}{c_j} \sum_{k \in \Gamma_j} (\partial_{n+1} \phi^{n+1})_{(j_1 k_1) \dots (j_n k_n)(jk)}(x_1, \dots, x_n, 0) \quad \forall j. \quad (91)$$

We have thus established a quantum field on a graph interacting with external sources in the vertices.

The minimal model still allowing to describe creation and annihilation of particles on graphs, i.e. the restriction to the 0-1-particle space \mathcal{F}_1^S , reads

$$\begin{aligned} (H\phi)_{jk}^1(x) &= -\phi_{jk}^1{}''(x), \\ (H\phi)^0 &= \sum_{j=1}^{N_v} \bar{c}_j \phi_{jk_j}^1(0) \quad \forall k_j \in \Gamma_j, \\ \text{with IBCs} \quad \phi^0 &= \frac{1}{c_j} \sum_{k \in \Gamma_j} \phi_{jk}^1{}'(0) \quad \forall j. \end{aligned} \quad (92)$$

In the limit $c_j \rightarrow 0$ the Fock space sectors decouple, as expected, and the IBCs reduce to a Kirchhoff boundary conditions in the one-particle sector.

The Hamiltonian (92) describes a particle which moves freely along the edges of a graph, can be annihilated whenever it reaches a vertex and can eventually be re-created at the same or at a different vertex. If re-creation of the particle always happened at the same vertex at which it was previously annihilated, we could alternatively think of the particle being trapped at this vertex for a certain period of time.² Modelling such a situation may be interesting in its own right, independently of our original motivation to describe particle creation and annihilation in the context of quantum field theory. In order to keep track of at which vertex the particle is trapped we replace the zero-particle wave function $\phi^0 \in \mathbb{C}$ by a vector $\phi^0 \in C^{N_v}$ with components ϕ_j^0 , one for each vertex. The modified model, which is no longer defined on $\mathcal{F}_1^S = \mathbb{C} \oplus \mathcal{H}$ but instead on $\mathbb{C}^{N_v} \oplus \mathcal{H}$, reads

$$\begin{aligned} (H\phi)_{jk}^1(x) &= -\phi_{jk}^1{}''(x), \\ (H\phi)_j^0 &= \bar{c}_j \phi_{jk}^1(0) \quad \forall k \in \Gamma_j, \\ \text{with IBCs} \quad \phi_j^0 &= \frac{1}{c_j} \sum_{k \in \Gamma_j} \phi_{jk}^1{}'(0). \end{aligned} \tag{93}$$

This last Hamiltonian is related to so-called quantum decorated graphs, see e.g. [36, 37] and references therein. A decorated graph is a metric graph, with each vertex replaced by a smooth manifold \mathcal{M}_j , $j = 1, \dots, N_v$. The Laplacian on a decorated graph is then defined on a suitable domain in

$$\left(\bigoplus_{j=1}^{N_v} L^2(\mathcal{M}_j) \right) \oplus \mathcal{H} \tag{94}$$

i.e. the direct sum of the L^2 -spaces over the vertex-manifolds and \mathcal{H} , which itself is the direct sum of the L^2 -spaces over the edges, see Eq. (82). Upon replacing each $L^2(\mathcal{M}_j)$ by \mathbb{C} , we obtain the Hilbert space of (93).

VII Conclusions and outlook

We have shown that the IBC-approach to particle creation and annihilation developed by Teufel and Tumulka [1, 2] in three spatial dimensions can also be applied to one-dimensional systems. We have presented an IBC-Hamiltonian on full Fock space and on a truncated Fock space, where at most one particle can be created. We have explicitly studied the characteristics of the 0-1-particle case as the minimal model for particle creation and annihilation in terms of IBCs. The IBC-Hamiltonian on full Fock space can also be studied in terms of explicit solutions; this we will discuss elsewhere. In the three-dimensional case Teufel and Tumulka introduce a whole family of different IBC-Hamiltonians. This is also possible in one dimension. For instance, one can essentially interchange the roles of ϕ^1 and $\phi^{1'}$ in (14) when allowing ϕ^1 to be discontinuous at the origin but demanding

²We owe this alternative interpretation to Stefan Teufel.

$\phi^{1'}(0+) = \phi^{1'}(0-)$. More general IBCs, involving linear combinations of ϕ^1 and $\phi^{1'}$, also lead to well-defined models. IBCs in two dimensions can also be defined, which will, e.g., allow to study particle creation and annihilation in quantum billiards. In the long run it will be interesting to see if realistic quantum field theories can be formulated non-perturbatively using IBCs. To this end it will be necessary to study quantised gauge fields and Dirac fermions in terms of IBCs.

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A Three-dimensional IBC-Hamiltonian

In Ref. [1] Teufel and Tumulka present an IBC appropriate to describe Schrödinger particles in three spatial dimensions which can be created and annihilated at an external source. They motivate their choice of IBC by discussing probability conservation on full Fock space. Here we show that the IBC of Ref. [1] can alternatively be motivated along the same lines as its one-dimensional analogue in Sec. II.

Now the single particle Hilbert space is $\mathcal{H} = L^2(\mathbb{R}^3)$, and $\mathcal{F}^S = P^S(\bigoplus_{n=0}^{\infty} \mathcal{H}^{\otimes n})$ as usual. Annihilation and creation operators $a(f)$ and $a^\dagger(f)$ are defined as in Eqs. (7) and (8). The starting point for our considerations is once more the tentative Hamiltonian (10) where now $y \in \mathbb{R}^3$. Again we write down the eigenvalue equation $H\phi = E\phi$ in the n -particle sector, cf. Eg. (11), integrate in x_n over the ball $B_r(y) = \{x_n \in \mathbb{R}^3 : |x_n - y| \leq r\}$ and subsequently take the limit $r \rightarrow 0+$, yielding

$$-\int_{B_r(y)} (\Delta_n \phi^n)(x_1, \dots, x_n) dx_n + \frac{c}{\sqrt{n}} \phi^{n-1}(x_1, \dots, x_{n-1}) = 0. \quad (95)$$

By applying Gauß' theorem, the first term can be rewritten as an integral over the two-sphere,

$$-\int_{B_r(y)} (\Delta_n \phi^n)(x_1, \dots, x_n) dx_n = -\int_{S^2} \frac{\partial \tilde{\phi}^n}{\partial r}(x_1, \dots, x_{n-1}, r, \omega) r^2 d\omega, \quad (96)$$

where we have introduced spherical coordinates $(r, \omega) \in [0, \infty) \times S^2$ centered at y through

$$\tilde{\phi}^n(x_1, \dots, x_{n-1}, r, \omega) = \phi^n(x_1, \dots, x_{n-1}, y + r\omega). \quad (97)$$

In the limit $r \rightarrow 0+$ the integral (96) vanishes for smooth functions ϕ^n . However, Teufel and Tumulka show [1] that when constructing the IBC-Hamiltonian one should include the

functions $ae^{-\kappa|x-y|}/|x-y|$, $a \in \mathbb{C}$, $\kappa > 0$, in the domain of the one-particle Hamiltonian. For these we have the non-zero result

$$-\int_{S^2} \left(\frac{\partial}{\partial r} a \frac{e^{-\kappa r}}{r} \right) r^2 d\omega = 4\pi a(\kappa r + 1)e^{-\kappa r} \xrightarrow{r \rightarrow 0+} 4\pi a. \quad (98)$$

Then again $\lim_{r \rightarrow 0+} (r \cdot ae^{-\kappa r}/r) = a$, whereas $\lim_{r \rightarrow 0+} r\phi^n(x_1, \dots, x_{n+1}, y+r\omega) = 0$ for continuous ϕ^n . Consequently,

$$-\lim_{r \rightarrow 0+} \int_{S^2} \frac{\partial \tilde{\phi}^n}{\partial r}(x_1, \dots, x_{n-1}, r, \omega) r^2 d\omega = 4\pi \lim_{r \rightarrow 0+} r\phi^n(x_1, \dots, x_{n-1}, y+r\omega), \quad (99)$$

which is the way in which this term is expressed within the IBC of Ref. [1]. Now we seem to have another problem. The Hamiltonian contains the term $a(\delta_y)$ but the functions $ae^{-\kappa|x-y|}/|x-y|$ cannot be evaluated at $x=y$. Here the way out is to notice that

$$\phi^n(x_1, \dots, x_{n-1}, y) = \lim_{r \rightarrow 0+} \frac{\partial}{\partial r} \left(r \tilde{\phi}^n(x_1, \dots, x_{n-1}, r, \omega) \right) \quad (100)$$

for smooth functions, and that the right-hand side is still defined for functions which diverge like $ae^{-\kappa|x_n-y|}/|x_n-y|$. Therefore, we have to redefine the annihilator according to

$$(a(\delta_y)\phi)^n(x_1, \dots, x_n) = \sqrt{n+1} \lim_{r \rightarrow 0+} \frac{\partial}{\partial r} \left(r \tilde{\phi}^{n+1}(x_1, \dots, x_n, r, \omega) \right). \quad (101)$$

Altogether, the Hamiltonian for the three-dimensional model reads, cf. [1],

$$H = -\Delta^{\mathcal{F}} + \bar{c} a(\delta_y) \quad (102)$$

with IBC $\phi^n(x_1, \dots, x_n) = -\frac{4\pi}{c} \sqrt{n+1} \lim_{r \rightarrow 0+} r \phi^{n+1}(x_1, \dots, x_n, y+r\omega).$

B Ground state in the limit of vanishing coupling

For vanishing coupling $c = 0$ the IBC-Hamiltonian (14) becomes the free Hamiltonian $H_{\text{free}} = -\Delta^{\mathcal{F}}$, i.e. $H_{\text{free}}(\phi^0, \phi^1) = (0, -\phi^{1''})$. Its ground state is the free vacuum $\phi_{\text{vac}} = (\phi_{\text{vac}}^0, \phi_{\text{vac}}^1) = (1, 0)$ with eigenvalue $E_{\text{vac}} = 0$. The ground state ϕ_g of the IBC-Hamiltonian for $c \neq 0$ is discussed in Sec.III, see Eq. (20). Naively, one would expect ϕ_g to approach ϕ_{vac} in the limit $c \rightarrow 0$, except for an arbitrary global phase. However, although $\lim_{c \rightarrow 0} E_g = E_{\text{vac}}$ and $\|\phi_g\|^2 = 1 \ \forall c \neq 0$ we observe

$$\lim_{c \rightarrow 0} \left(-\frac{c}{|c|} \phi_g \right) = \left(\sqrt{\frac{2}{3}}, 0 \right), \quad (103)$$

and in particular $\|\lim_{c \rightarrow 0} \phi_g\|^2 = 2/3 \neq \lim_{c \rightarrow 0} \|\phi_g\|^2$.

This artefact is a remnant of an infrared divergence which would appear for the IBC-Hamiltonian on full Fock space. Even for small couplings the energy of ϕ_{vac} can be lowered

by creating a small kink in the one-particle sector at the position of the source. Although ϕ_g^1 decays exponentially, the decay rate decreases with decreasing coupling constant c . Physically, this means that with decreasing coupling the particle cloud surrounding the source delocalises more and more, and ultimately the particle partially escapes to infinity. This can be seen as follows. The expectation value of the particle vanishes, $\langle \phi_g^1, x \phi_g^1 \rangle_{L^2(\mathbb{R})} = 0 \ \forall c$, since ϕ_g^1 is symmetric. The variance, however, diverges when the coupling goes to zero,

$$\langle \phi_g^1, x^2 \phi_g^1 \rangle_{L^2(\mathbb{R})} = \frac{\kappa}{3} \int_{-\infty}^{\infty} e^{-2\kappa|x|} dx = \frac{1}{6\kappa^2} \xrightarrow{|c| \rightarrow 0} \infty. \quad (104)$$

In order to recover the free vacuum in the limit of vanishing coupling, we have to first add a zero point energy $M > 0$ (“rest mass”), which is only removed after the limit $c \rightarrow 0$. The modified IBC-Hamiltonian, cf. Eq. (14) then reads

$$(H\phi)^1 = -\phi^{1''} + M\phi^1, \quad (H\phi)^0 = \bar{c}\phi^1(0) \quad \text{with IBC} \quad \phi^0 = \frac{1}{c} \left[\phi^{1'}(x) \right]_{x=0-}^{x=0+}. \quad (105)$$

For the ground state we again make the ansatz $\phi^1(x) = A \exp(-\kappa|x|)$, $\kappa > 0$. From the eigenvalue equation in the one-particle sector we can read off the energy $E = -\kappa^2 + M$. In the zero-particle sector the eigenvalue equation yields $\bar{c}A = E\phi^0 \Leftrightarrow \phi^0 = \bar{c}A/(-\kappa^2 + M)$ and the IBC reads $\phi^0 = -2A\kappa/c$. The last two conditions can only be satisfied if $\kappa^2 > M$, and then κ has to solve

$$2\kappa(\kappa^2 - M) = |c|^2. \quad (106)$$

The normalisation condition $\|\phi\|^2 = 1$ requires $|A| = \sqrt{\kappa \frac{\kappa^2 - M}{3\kappa^2 - M}}$ implying

$$|\phi^0|^2 = \frac{2\kappa^2}{3\kappa^2 - M} \quad \text{and} \quad \|\phi^1\|^2 = \frac{\kappa^2 - M}{3\kappa^2 - M}. \quad (107)$$

Fulfilling condition (106) under the constraint $\kappa^2 > M$ requires that $\kappa \rightarrow \sqrt{M}+$ when $|c| \rightarrow 0$, and thus

$$|\phi^0|^2 \xrightarrow{|c| \rightarrow 0} 1 \quad \text{and} \quad \|\phi^1\|^2 \xrightarrow{|c| \rightarrow 0} 0. \quad (108)$$

Hence, except for the undetermined phase, we recover the free vacuum $(\phi_{\text{vac}}^0, \phi_{\text{vac}}^1) = (1, 0)$.

C Orthonormality and completeness of the eigenstates

Orthonormality. We show that $\langle \phi_g, \phi_k \rangle = 0$ and $\langle \phi'_k, \phi_k \rangle = \delta(k - k')$ for the eigenstates ϕ_g and ϕ_k which are given in (20), (22), (23) and (24). For the first relation we consider

$$\overline{\phi_g^0} \phi_k^0 = -\sqrt{\frac{2}{3\pi}} \frac{\sqrt{k^2 \kappa^3}}{|k|^3 + i\kappa^3}, \quad (109)$$

and

$$\begin{aligned}
\int_{-\infty}^{\infty} \overline{\phi_g^1(x)} \phi_k^1(x) dx &= \int_{-\infty}^{\infty} \sqrt{\frac{\kappa}{3}} e^{-\kappa|x|} \frac{1}{\sqrt{2\pi}} (e^{ikx} + b_k e^{i|k||x|}) dx \\
&= \sqrt{\frac{\kappa}{6\pi}} \left[\frac{1}{\kappa - ik} + \frac{1}{\kappa + ik} + \frac{(-2i\kappa^3)}{(\kappa - i|k|)(|k|^3 + i\kappa^3)} \right] \\
&= \sqrt{\frac{\kappa}{6\pi}} \frac{2\kappa|k|^3 + 2\kappa^3|k|}{(\kappa^2 + k^2)(|k|^3 + i\kappa^3)} \\
&= \sqrt{\frac{2}{3\pi}} \frac{\sqrt{k^2 \kappa^3}}{|k|^3 + i\kappa^3}.
\end{aligned} \tag{110}$$

Adding both results shows that $\langle \phi_g, \phi_k \rangle = 0$ for all $k \in \mathbb{R}$.

For the inner product between two scattering states we consider

$$\overline{\phi_{k'}^0} \phi_k^0 = \frac{2|kk'|}{\pi|c|^2} \overline{b_{k'}} b_k = \frac{|k'k| \kappa^3}{\pi(|k|^3 + i\kappa^3)(|k'|^3 - i\kappa^3)}, \tag{111}$$

and

$$\begin{aligned}
\int_{-\infty}^{\infty} \overline{\phi_{k'}^1(x)} \phi_k^1(x) dx &= \frac{1}{2\pi} \int_{-\infty}^{\infty} [e^{-ik'x} + \overline{b_{k'}} e^{-i|k'||x|}] [e^{ikx} + b_k e^{i|k||x|}] dx \\
&= \delta(k - k') + \frac{1}{2\pi} \left[\frac{i \overline{b_{k'}}}{k - |k'| + i0+} + \frac{i \overline{b_{k'}}}{-k - |k'| + i0+} \right. \\
&\quad \left. + \frac{i b_k}{-k' + |k| + i0+} + \frac{i b_k}{k' + |k| + i0+} + \frac{2i b_k \overline{b_{k'}}}{|k| - |k'| + i0+} \right],
\end{aligned} \tag{112}$$

where we have used the identity (see e.g. Appendix II of [38])

$$\int_0^{\infty} e^{ikx} dx = \frac{i}{k + i0+} = \pi \delta(k) + \mathcal{P} \frac{i}{k}. \tag{113}$$

Here \mathcal{P} stands for principal value. The expression in the square bracket in the final equality of (112) is even in k and in k' . We assume in the following $k, k' > 0$ and we later use the evenness to extend the result to all real values of k and k' .

$$\begin{aligned}
\int_{-\infty}^{\infty} \overline{\phi_{k'}^1(x)} \phi_k^1(x) dx &= \delta(k - k') + \frac{i}{2\pi} \frac{(b_k + \overline{b_{k'}} + 2b_k \overline{b_{k'}})}{k - k' + i0+} + \frac{i}{2\pi} \frac{(b_k - \overline{b_{k'}})}{k + k'} \\
&= \delta(k - k') - \frac{\kappa^3(k^2 + kk' + k'^2)}{2\pi(k^3 + i\kappa^3)(k'^3 - i\kappa^3)} + \frac{\kappa^3(k^2 - kk' + k'^2)}{2\pi(k^3 + i\kappa^3)(k'^3 - i\kappa^3)} \\
&= \delta(k - k') - \frac{k'k \kappa^3}{\pi(k^3 + i\kappa^3)(k'^3 - i\kappa^3)}.
\end{aligned} \tag{114}$$

The result is extended to $k, k' \in \mathbb{R}$ by replacing k by $|k|$ and k' by $|k'|$ in the fraction. Combining the result (114) with (111) shows that $\langle \phi_{k'}, \phi_k \rangle = \delta(k - k')$ for all $k, k' \in \mathbb{R}$.

Completeness. We showed in section III that completeness requires the three relations

$$|\phi_g^0|^2 + \int_{-\infty}^{\infty} |\phi_k^0|^2 dk = 1, \quad (115)$$

$$\overline{\phi_g^0} \phi_g^1(x) + \int_{-\infty}^{\infty} \overline{\phi_k^0} \phi_k^1(x) dk = 0, \quad (116)$$

$$\overline{\phi_g^1(y)} \phi_g^1(x) + \int_{-\infty}^{\infty} \overline{\phi_k^1(y)} \phi_k^1(x) dk = \delta(x - y). \quad (117)$$

The derivations are similar to that for a delta-potential [39]. Starting with (115), we obtain

$$|\phi_g^0|^2 + \int_{-\infty}^{\infty} |\phi_k^0|^2 dk = \frac{2}{3} + \int_{-\infty}^{\infty} \frac{|k b_k|^2}{\pi \kappa^3} dk = \frac{2}{3} + \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{k^2 \kappa^3}{k^6 + \kappa^6} dk = 1. \quad (118)$$

For the second relation (116) we consider

$$\overline{\phi_g^0} \phi_g^1(x) = -\frac{\sqrt{2\kappa}}{3} e^{-\kappa|x|} e^{i\varphi_c}, \quad (119)$$

and

$$\int_{-\infty}^{\infty} \overline{\phi_k^0} \phi_k^1(x) dk = \int_{-\infty}^{\infty} \sqrt{\frac{k^2 \kappa^3}{2\pi^2}} \frac{e^{i\varphi_c}}{|k|^3 - i\kappa^3} \left[e^{ikx} + \frac{-i\kappa^3}{|k|^3 + i\kappa^3} e^{i|k||x|} \right] dk. \quad (120)$$

Applying Euler's formula $e^{ikx} = \cos(kx) + i\sin(kx)$ shows that only the cosine term contributes and that the expression is even in x . Hence we may assume $x \geq 0$ in the following and later replace x by $|x|$ to extend the result to all $x \in \mathbb{R}$. Furthermore, we use evenness in k to integrate only over positive values of k . After inserting Euler's formula also for the second exponential in the square bracket we obtain

$$\begin{aligned} \int_{-\infty}^{\infty} \overline{\phi_k^0} \phi_k^1(x) dk &= \frac{\sqrt{2\kappa^3}}{\pi} e^{i\varphi_c} \int_0^{\infty} \frac{k}{k^6 + \kappa^6} [k^3 \cos(kx) + \kappa^3 \sin(kx)] dk \\ &= \frac{\sqrt{2\kappa^3}}{4\pi} e^{i\varphi_c} \int_{-\infty}^{\infty} \frac{k}{k^6 + \kappa^6} [(k^3 - i\kappa^3)e^{ikx} + (k^3 + i\kappa^3)e^{-ikx}] dk \\ &= \frac{\sqrt{2\kappa^3}}{2\pi} e^{i\varphi_c} \int_{-\infty}^{\infty} \frac{k}{k^3 + i\kappa^3} e^{ikx} dk \\ &= \frac{\sqrt{2\kappa}}{3} e^{-\kappa x} e^{i\varphi_c}. \end{aligned} \quad (121)$$

The integral was evaluated by contour integration around the pole in the upper half plane at $k = i\kappa$. The result is extended to $x \in \mathbb{R}$ by replacing x by $|x|$. Combining the result with (119) confirms the second relation (116).

For the third relation (117) we consider

$$\overline{\phi_g^1(y)} \phi_g^1(x) = \frac{\kappa}{3} e^{-\kappa(|x|+|y|)}, \quad (122)$$

and

$$\begin{aligned} \int_{-\infty}^{\infty} \overline{\phi_k^1(y)} \phi_k^1(x) dk &= \frac{1}{2\pi} \int_{-\infty}^{\infty} [e^{ikx} + b_k e^{i|k||x|}] [e^{-iky} + \overline{b_k} e^{-i|k||y|}] dk \\ &= \delta(x-y) + \frac{\kappa^3}{2\pi} (I_1(x,y) + I_2(x,y) + I_3(x,y)) , \end{aligned} \quad (123)$$

where

$$I_1(x,y) = i \int_{-\infty}^{\infty} \frac{1}{|k|^3 - i\kappa^3} e^{ikx} e^{-i|k||y|} dk , \quad I_3(x,y) = \int_{-\infty}^{\infty} \frac{\kappa^3}{k^6 + \kappa^6} e^{i|k||x|} e^{-i|k||y|} dk , \quad (124)$$

and $I_2(x,y) = \overline{I_1(y,x)}$. Using Euler's formula $e^{ikx} = \cos(kx) + i \sin(kx)$ for $I_1(x,y)$ shows that only the cosine term contributes. It shows further that $I_1(x,y)$ is even in x and in y and that its integrand is even in k . The same holds for $I_2(x,y)$ and $I_3(x,y)$. We assume $x, y \geq 0$ in the following and restrict the integrals to positive values of k . We bring all fractions onto the denominator $(k^6 + \kappa^6)$ and obtain

$$\begin{aligned} I_1(x,y) &= \int_0^{\infty} \frac{2 \cos(kx)}{k^6 + \kappa^6} [(k^3 \sin(ky) - \kappa^3 \cos(ky)) + i (k^3 \cos(ky) + \kappa^3 \sin(ky))] dk , \\ I_2(x,y) &= \int_0^{\infty} \frac{2 \cos(ky)}{k^6 + \kappa^6} [(k^3 \sin(kx) - \kappa^3 \cos(kx)) - i (k^3 \cos(kx) + \kappa^3 \sin(kx))] dk , \\ I_3(x,y) &= \int_0^{\infty} \frac{2\kappa^3}{k^6 + \kappa^6} [\cos(k(x-y)) + i \sin(k(x-y))] dk . \end{aligned} \quad (125)$$

After adding all three terms the imaginary part vanishes and the real part gives

$$\begin{aligned} I_1(x,y) + I_2(x,y) + I_3(x,y) &= \int_0^{\infty} \frac{2}{k^6 + \kappa^6} [k^3 \sin(k(x+y)) - \kappa^3 \cos(k(x+y))] dk \\ &= -\frac{i}{2} \int_{-\infty}^{\infty} \left[\frac{k^3 - i\kappa^3}{k^6 + \kappa^6} e^{ik(x+y)} - \frac{k^3 + i\kappa^3}{k^6 + \kappa^6} e^{-ik(x+y)} \right] dk \\ &= -i \int_{-\infty}^{\infty} \frac{1}{k^3 + i\kappa^3} e^{ik(x+y)} dk \\ &= -\frac{2\pi}{3\kappa^2} e^{-\kappa(x+y)} . \end{aligned} \quad (126)$$

The integral was evaluated by contour integration in the upper half plane around the pole at $k = i\kappa$. The result can be extended to $x, y \in \mathbb{R}$ by replacing x by $|x|$ and y by $|y|$. Combining the result with (122) and (123) shows (117).

D Time evolution kernel

This section contains a derivation of the time evolution kernel of the IBC-Hamiltonian (14), based on an eigenfunction expansion. Alternatively, the kernel can also be obtained from

a Fourier-Laplace transform of the Green function in (33) and (34), leading to the same result.

The eigenfunction expansion of the time evolution operator $K(T) = e^{-iHT}$ has the form

$$K(T) = \phi_g \langle \phi_g, \cdot \rangle e^{i\kappa^2 T} + \int_{-\infty}^{\infty} \phi_k \langle \phi_k, \cdot \rangle e^{-ik^2 T} dk,$$

and the eigenstates are given in (20), (22) and (23).

We consider first the 11-sector. After inserting the eigenfunctions ϕ_g^1 and ϕ_k^1 we obtain the integral kernel

$$K^{11}(x, y, T) = \frac{\kappa}{3} e^{-\kappa(|x|+|y|)} e^{i\kappa^2 T} + K_0^{11}(x, y, T) + \frac{\kappa^3}{2\pi} (I_1(x, y, T) + I_2(x, y, T) + I_3(x, y, T)), \quad (127)$$

where

$$K_0(x, y, T) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ik^2 T} e^{ik(x-y)} dk = \frac{1}{\sqrt{4\pi i T}} \exp\left(-\frac{(x-y)^2}{4iT}\right), \quad (128)$$

is the free time evolution kernel in single-particle quantum mechanics, and

$$\begin{aligned} I_1(x, y, T) &= i \int_{-\infty}^{\infty} \frac{1}{|k|^3 - i\kappa^3} e^{ikx} e^{-i|k||y|} e^{-ik^2 T} dk, \\ I_2(x, y, T) &= -i \int_{-\infty}^{\infty} \frac{1}{|k|^3 + i\kappa^3} e^{-iky} e^{i|k||x|} e^{-ik^2 T} dk, \\ I_3(x, y, T) &= \int_{-\infty}^{\infty} \frac{\kappa^3}{k^6 + \kappa^6} e^{i|k||x|} e^{-i|k||y|} e^{-ik^2 T} dk. \end{aligned} \quad (129)$$

Note that the functions I_j differ from those in (124) only by the additional term $e^{-ik^2 T}$ in the integrand. The calculations are completely analogous to those from (124) to (126) and lead to

$$I_1(x, y, T) + I_2(x, y, T) + I_3(x, y, T) = -i \int_{-\infty}^{\infty} \frac{1}{k^3 + i\kappa^3} e^{ik(|x|+|y|)} e^{-ik^2 T} dk. \quad (130)$$

The integral can be evaluated after applying the partial fraction expansion

$$\frac{1}{k^3 + i\kappa^3} = -\frac{1}{3\kappa^3} \left[\frac{\kappa_0}{k - i\kappa_0} + \frac{\kappa_1}{k - i\kappa_1} + \frac{\kappa_2}{k - i\kappa_2} \right], \quad (131)$$

where $\kappa_j = \kappa \exp(2\pi i j/3)$ for $j = 0, 1, 2$. Note that a useful formula is (for $n \in \mathbb{Z}$)

$$\sum_{j=0}^2 \kappa_j^n = \begin{cases} 3\kappa^n & \text{if } n \text{ is divisible by } 3, \\ 0 & \text{otherwise.} \end{cases} \quad (132)$$

After inserting the partial fraction expansion into (130), the resulting integral can be evaluated with the formula

$$\int_{-\infty}^{\infty} \frac{\exp(-\beta z^2 + i\alpha z)}{z \mp i\gamma} dz = \pm i\pi \exp(\beta\gamma^2 \mp \alpha\gamma) \operatorname{erfc}\left(\sqrt{\beta}\gamma \mp \frac{\alpha}{2\sqrt{\beta}}\right), \quad (133)$$

where $\text{Re } \alpha > 0$, $\text{Re } \beta \geq 0$, $\text{Re } \gamma > 0$ and erfc is the complementary error function. Equation (133) can be obtained, for example, by using

$$\frac{1}{z \mp i\gamma} = \pm i \int_0^\infty dt \exp(\mp i(z \mp i\gamma)t).$$

After applying the integral (133) one finally obtains the result for the time evolution kernel

$$K^{11}(x, y, T) = K_0^{11}(x, y, T) + \sum_{j=0}^2 \frac{\kappa_j}{6} e^{i\kappa_j^2 T} e^{-\kappa_j(|x|+|y|)} \text{erfc}\left(\frac{|x|+|y|}{2\sqrt{iT}} - \kappa_j\sqrt{iT}\right). \quad (134)$$

The ground state contribution in (127) has been included here in the $j = 0$ term. Equation (134) is the final result for the time evolution kernel. It can be expressed in an alternative form that can be obtained after inserting the integral representation of the error-function and changing the integration variable

$$K^{11}(x, y, T) = K_0(x, y, T) + \sum_{j=0}^2 \frac{\kappa_j}{3} \int_0^\infty e^{\kappa_j u} K_0(|x| + |y| + u, 0, T) du. \quad (135)$$

There are again similarities to the time evolution kernel for a delta-potential [40, 41].

The expressions for the kernel in the other sectors can be obtained from the eigenfunction expansion in these sectors, or alternatively by applying the IBCs to $K^{11}(x, y, T)$. We give here only the results

$$\begin{aligned} K^{10}(x, T) &= - \sum_{j=0}^2 \frac{\kappa_j^2}{3\bar{c}} e^{i\kappa_j^2 T} e^{-\kappa_j|x|} \text{erfc}\left(\frac{|x|}{2\sqrt{iT}} - \kappa_j\sqrt{iT}\right), \\ K^{01}(y, T) &= - \sum_{j=0}^2 \frac{\kappa_j^2}{3c} e^{i\kappa_j^2 T} e^{-\kappa_j|y|} \text{erfc}\left(\frac{|y|}{2\sqrt{iT}} - \kappa_j\sqrt{iT}\right), \\ K^{00}(T) &= \frac{1}{3} \sum_{j=0}^2 e^{i\kappa_j^2 T} \text{erfc}(-\kappa_j\sqrt{iT}). \end{aligned} \quad (136)$$

In Sec. III we use the long-time behaviour of $K^{00}(T)$. It can be obtained from the asymptotics of the erfc -function

$$\text{erfc}(z) = \frac{\exp(-z^2)}{\sqrt{\pi}z} \left(1 - \frac{1}{(2z^2)} + \frac{1 \cdot 3}{(2z^2)^2} + \dots\right) \quad \text{as } |z| \rightarrow \infty, |\arg z| < \frac{3\pi}{4}. \quad (137)$$

In the remaining sector of $\arg z$ one has to add a 2 to the asymptotic expansion. Using (137) and (132) one finds

$$K^{00}(T) = \frac{2}{3} e^{i\kappa^2 T} + \mathcal{O}(T^{-3/2}) \quad \text{as } T \rightarrow \infty. \quad (138)$$

The short-time behaviour of the time evolution kernel is supposed to reveal the underlying classical dynamics, see e.g. [16]. For K^{00} a Taylor expansion yields $K^{00}(T) = 1 + \mathcal{O}(T^{3/2})$. The phases of the arguments of the error functions in the other three components all approach $-\frac{\pi}{4}$ for small T . Thus, we can use the asymptotics (137), and performing the j -sum with the help of Eq. (132) yields

$$\begin{aligned} K^{11}(x, y, T) &= K_0(x, y, T) - \frac{4i|c|^2 T^3}{(|x| + |y|)^3} \frac{\exp\left(-\frac{(|x|+|y|)^2}{4iT}\right)}{\sqrt{4\pi iT}} (1 + \mathcal{O}(T)), \\ K^{10}(x, T) &= \frac{2c T^2}{|x|^2} \frac{\exp\left(-\frac{|x|^2}{4iT}\right)}{\sqrt{4\pi iT}} (1 + \mathcal{O}(T)), \\ K^{01}(y, T) &= \frac{2\bar{c} T^2}{|y|^2} \frac{\exp\left(-\frac{|y|^2}{4iT}\right)}{\sqrt{4\pi iT}} (1 + \mathcal{O}(T)). \end{aligned} \tag{139}$$

These results can be understood in a similar way as the Green function in Sec III. K^{11} , in addition to the direct term K_0 , contains a diffractive contribution which can be associated with a path of length $|x|+|y|$. We interpret this term as coming from a particle moving from y to the origin, where it is annihilated, subsequently re-created, and which then moves on to x . The dependence on the coupling, $|c|^2$ is consistent with annihilation, proportional to \bar{c} , and subsequent re-creation, yielding a factor c . We also observe that the diffractive contribution decreases with increasing $(|x|+|y|)/T$, the mean velocity along the path. Thus, only slow particles couple strongly to the source. Similar interpretations apply for K^{10} and K^{01} .

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